Finite Element Method applied to the Fractional Partial Derivative Equation of Anomalous Diffusion

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Abstract. Diffusion, a fundamental phenomenon in natural processes, occurs on both microscopic and macroscopic scales. At the microscopic level, it manifests itself as a stochastic process, while at the macroscopic level it represents a uniform drift towards equilibrium. Fick's second law equation is widely used to model diffusion phenomena in various disciplines, including physics, chemistry, biology, and others. However, the classical Fick's law cannot correctly describe the movement of species through inhomogeneous materials, such as porous media. This phenomenon is known as non-Fickian or anomalous diffusion and presents behavior that is challenging to analyze, requiring the use of computationally intensive simulations. To address this, recent studies have explored modeling anomalous diffusion using fractional derivatives in time or space. Fractional calculus, a branch of classical calculus, provides a framework for handling integrals and derivatives of arbitrary order. Its application has proven to be particularly effective in systems that exhibit hysteresis, allowing the computation of associated memory effects. One example is the modeling of anomalous diffusion in polymeric coatings used to protect flexible pipelines in subsea oil exploration. Under such adverse conditions, extreme depths and temperatures, the properties of the polymer change over time, affecting the ingress of corrosive ions into the metal structure. It left unchecked, this threatens operational safety and environmental integrity. In this work, the Finite Element Method (FEM) is applied to anomalous diffusion described by Fractional Partial Derivative Equations (FPDEs) in order to begin to understand these intricate transport dynamics.

Keywords: Anomalous Diffusion, Fractional Calculus, Finite Element Method, Polymeric coatings.

1 Introduction

Diffusion is a natural phenomenon that describes the spread of any quantity or species from regions of high concentration to low concentration, characterizing the evolution of non-equilibrium systems towards equilibrium. Classical diffusion, as postulated by Fick's law, assumes linear relationships between the mean square displacement of particles and time. Furthermore, the Brownian motion, which is modelled by the random walk results in a symmetrical curve behavior, a Gaussian distribution, as mentioned by Oliveira et al. [1]. However, anomalous diffusion deviates from these classical expectations and is often observed in complex and inhomogeneous systems with spatial heterogeneities or fractal structures that restrain or facilitate movement, such as porous materials. Every solid or condensed matter can virtually be treated as a porous medium (Tartakovsky and Dents [2]).

Fractional calculus allows the representation of this non-Gaussian statistical process, so called anomalous transport, whose mean square displacement in respect of time is characterized by $\langle \Delta x \rangle^2 \propto t^{\alpha}$, where the value of α varies from $0 < \alpha < 1$; $\alpha = 1$ or $\alpha > 1$, defining the sub, ideal and super diffusion, respectively (Lenzi et al.

[3]).

As noted by Ali et al. [4], over the years, numerous fractional derivatives have been proposed, notably the Riemann-Liouville, Grunwald-Letnikov and Caputo operators, and interest in this branch of calculus is growing due to its ability to predict history dependent problems. The Riemann-Liouville definition is often used in more mathematical treatises, while the Caputo derivative is preferred to model real problems due to its capacity to adequately describe some initial and boundary conditions, as pointed out by Luchko [5]. Studies of Tateishi et al. [6] and Concezzi and Spigler [7] confirm the importance of the time fractional derivative to better simulate anomalous diffusion in complex porous systems.

While many analytical procedures have been proposed to model fractional partial derivative equations (FPDEs), this paper focuses on solving the anomalous diffusion problem described by a fractional derivative in Caputo sense using the Finite Element Method (FEM).

2 FEM Formulation

2.1 Fickian Diffusion

The Fick's second law of diffusion for one dimension with a constant diffusion coefficient is defined by:

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2} \tag{1}$$

where $u(x,t)$ is the concentration in (mol/m³) and D is the diffusion coefficient in (m²/s). Appling the Galerkin method, as presented by Zienkiewicz and Taylor [8], in the eq. (1) results the semi discrete approximation given by:

$$\boldsymbol{M}\frac{\partial u}{\partial t} + \boldsymbol{K}\boldsymbol{u} = \boldsymbol{f} \tag{2}$$

$$\boldsymbol{M} = \int_{\Omega} \boldsymbol{N}^T\boldsymbol{N}\, d\Omega \tag{3}$$

$$\boldsymbol{K} = D\int_{\Omega} \boldsymbol{B}^T\boldsymbol{B}\, d\Omega \tag{4}$$

$$\boldsymbol{f} = \int_{\Gamma} \boldsymbol{N}^T\boldsymbol{q}\, d\Gamma \tag{5}$$

where $\boldsymbol{M}$ is the mass matrix described in eq. (3), $\boldsymbol{K}$ is the stiffness matrix described in eq. (4), $\boldsymbol{f}$ is the load vector described in eq. (5) and $\boldsymbol{u}$ is the nodal concentrations vector. The matrix $\boldsymbol{N}$ corresponds to the arbitrary shape functions, usually linear Lagrange polynomials, the matrix $\boldsymbol{B}$ to their respective derivatives, and the vector $\boldsymbol{q}$ contains the prescribed fluxes. Considering now a time discretization in eq. (2) assuming a linear variation of $\boldsymbol{u}$ between the times t_n and t_{n+1}, by Taylor series truncated in the first term, we get:

$$\left(\frac{\boldsymbol{M}}{\Delta t} + \theta\boldsymbol{K}\right)\boldsymbol{u}_{n+1} = \boldsymbol{f} - \left[(1-\theta)\boldsymbol{K} - \frac{\boldsymbol{M}}{\Delta t}\right]\boldsymbol{u}_n \tag{6}$$

where $\Delta t = t_{n+1} - t_n$, $\boldsymbol{u}_{n+1} = \boldsymbol{u}(t_{n+1})$ and $\boldsymbol{u}_n = \boldsymbol{u}(t_n)$.

The θ parameter describes the method used in the time iteration as follows: $\theta = 0$ corresponds to the explicit Euler method; $\theta = 0.5$ corresponds to Crank-Nicolson method; $\theta = 0.67$ corresponds to Galerkin method and $\theta = 1$ corresponds to the backward difference, as mentioned by Zienkiewicz and Taylor [8].

2.2 Anomalous Diffusion by Fractional Derivative

In the study of Ciesielski and Leszezynski [9], a FPDE in Caputo sense for a non-Fickian diffusion can be described as:

$$\frac{\partial_C^\alpha u(x,t)}{\partial t^\alpha} = D\frac{\partial^2 u(x,t)}{\partial x^2} \tag{7}$$

According to Ali et al. [4], the definition of the Caputo derivative for an arbitrary order of α is:

$$\frac{\partial_C^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{1}{(t-\tau)^\alpha}\frac{\partial u(x,t)}{\partial \tau}\,d\tau \tag{8}$$

where $\Gamma(\cdot)$ is the Gamma function. Following the same steps presented in the FEM formulation for the ideal diffusion, we obtain:

$$\boldsymbol{M}\frac{\partial_C^\alpha u}{\partial t} + \boldsymbol{K}\boldsymbol{u} = \boldsymbol{f} \tag{9}$$

Correa et al. [10] and Ammi et al. [11] demonstrated that the fractional derivative can be computed analytically after the linear discretization of $\boldsymbol{u}$ with respect to τ in eq. (8), resulting in a discrete form given by:

$$\frac{\partial_C^\alpha \boldsymbol{u}}{\partial t^\alpha} = \frac{1}{\Gamma(2-\alpha)\Delta t^\alpha}\left\{(\boldsymbol{u}_{n+1} - \boldsymbol{u}_n) + \sum_{j=0}^{n-1}[(n+1-j)^{1-\alpha} - (n-j)^{1-\alpha}](\boldsymbol{u}_{j+1} - \boldsymbol{u}_j)\right\} \tag{10}$$

Equation (10) now can be substituted into eq. (9) assuming $\boldsymbol{u} = \boldsymbol{u}_{n+1}$ and rearranging provides:

$$(G\boldsymbol{M} + \boldsymbol{K})\boldsymbol{u}_{n+1} = \boldsymbol{f} + G\boldsymbol{M}\left[\boldsymbol{u}_n - \sum_{j=0}^{n-1}\beta(\boldsymbol{u}_{j+1} - \boldsymbol{u}_j)\right] \tag{11}$$

where:

$$G = \frac{1}{\Gamma(2-\alpha)\Delta t^\alpha} \tag{12}$$

$$\beta = (n+1-j)^{1-\alpha} - (n-j)^{1-\alpha} \tag{13}$$

It is worth mentioning that the summation term in eq. (10) represents the non-locality or memory effect of the fractional derivative and implies in that every new step of $\boldsymbol{u}$ must consider the history contribution. In eq. (11) the β factor is zero when $\alpha = 1$, which corresponds to the classical diffusion of eq. (6) for $\theta = 1$.

3 Case study

In offshore oil exploration, flexible pipelines are composed of various metal structures and multi-layer polymer coatings, predominantly polyamide (PA 11). Cathodic protection is also applied to these pipelines to mitigate any corrosive environment that may be formed in the annular region due to gas and water permeation through the coatings. Mass transport from the inner region is complex in many ways, but the high temperatures can allow Fick's law to describe the interaction between the polymer and the penetrant. Externally, however, the deep seawater is around 4 °C. This means that the external region in contact with the PA 11 layer has a temperature lower than the glass transition temperature of the polymer (42 ºC). Under these conditions, the diffusion of species through the polymeric layer tends to be anomalous or non-Fickian (Karimi [12]).

This problem motivated the study of a simple 1D case to begin an analysis of the effects of the time fractional operator in a known ideal solution. This paper considers water uptake and diffusion in a polyamide 11 coating below the glass transition temperature, which characterizes a sub-diffusion problem. According to Razumovskii et al. [13], the average diffusion coefficient in this case is about $D = 3 \times 10^{-13}\ m^2/s$.

3.1 Diffusion in a Semi-Infinite Domain

To investigate the influence of the order of the fractional derivative in the diffusion phenomenon, an 1D semi-infinite domain with a prescribed concentration in $x = 0$ in the time $t = 0$ is analyzed.

The problem corresponds to the eq. (1) with the initial and boundary conditions given by:

$$u(0,t) = u_0, \quad u(\infty,t) = 0, \quad u(x,0) = 0\,, \qquad \forall\, x > 0 \tag{14}$$

The analytical solution of this problem is presented by Crank [14] as:

$$u(x,t) = u_0\left[1 - efr\left(\frac{x}{2\sqrt{Dt}}\right)\right] \tag{15}$$

where $efr(\cdot)$ is the Gauss error function. To replicate the analytical solution, a FEM simulation was performed using the ideal diffusion formulation of eq. (6) to analyze a domain of 1 mm discretized by a mesh of 500 elements. The infinite domain was represented by an additional domain of 1 m discretized by a mesh of 50 elements, and the calculations assumed a total time of 48 hours with time steps of 450 seconds. The boundary concentration at $x = 0$ was set to 100 mol/m³, with no prescribed flux. The time iteration was performed considering the θ parameter equal to one. Figure 1 shows the concentration profiles along the position x for different times obtained from an implemented FEM Python code and considering the ideal Fickian diffusion.

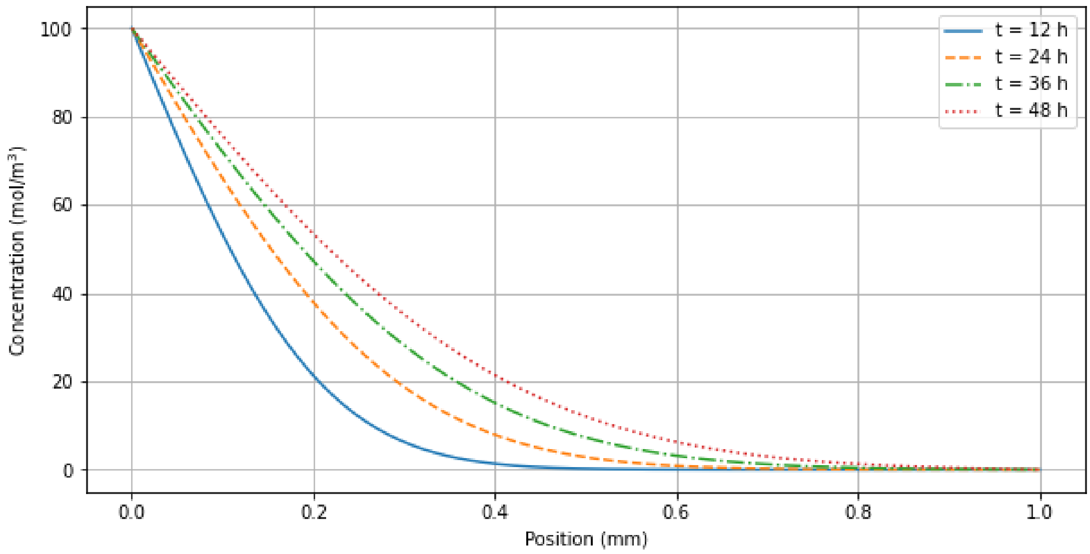

Figure 1. Concentration profiles of the ideal Fickian diffusion for different times.

The results correspond exactly to the analytical solution of eq. (15) for the given times, confirming that the mesh size and time steps are sufficient to describe the semi-infinite domain problem. The next step was to implement the FEM formulation of the anomalous diffusion presented in eq. (11) with the same mesh size and time steps.

In the sub diffusive case, the motion of the molecules takes a long time to evolve, so to visualize the effect of the fractional order derivative, the time point plotted in Fig. 2, which shows the behavior of these profiles as α varies between 0.75 and 1, was set to 48 hours. The concentration profile when $\alpha = 1$ must correspond to that in Fig. 1 at 48 h.

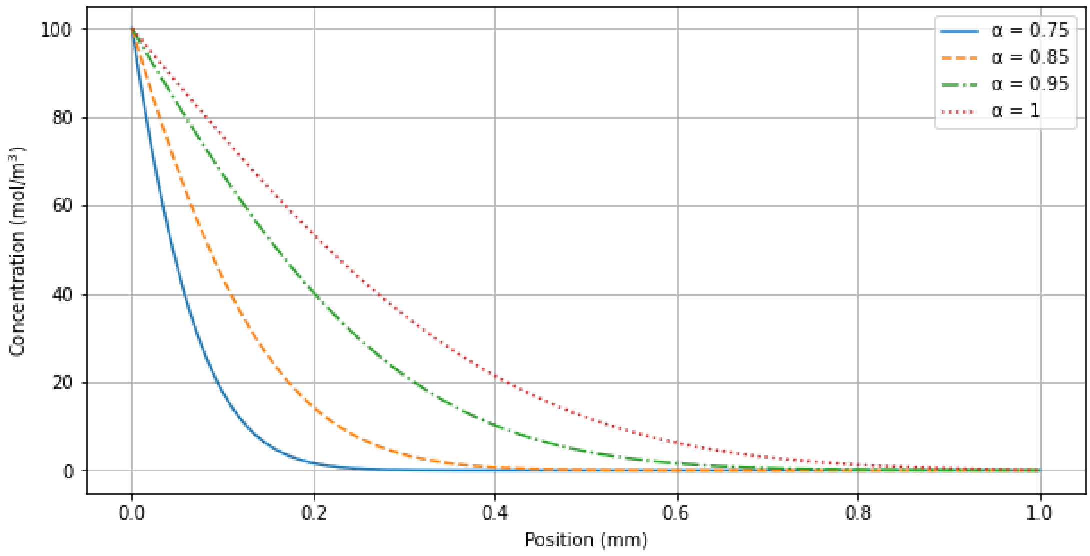

Figure 2. Concentration profiles for different α fractional order at 48 h.

As expected, the dotted line in Fig. 2 is the same as in Fig. 1 and represents ideal diffusion. For lower values of α, the diffusion is so slow that to better visualization, just 0.1 mm (10%) of the analyzed domain is plotted in Fig. 3.

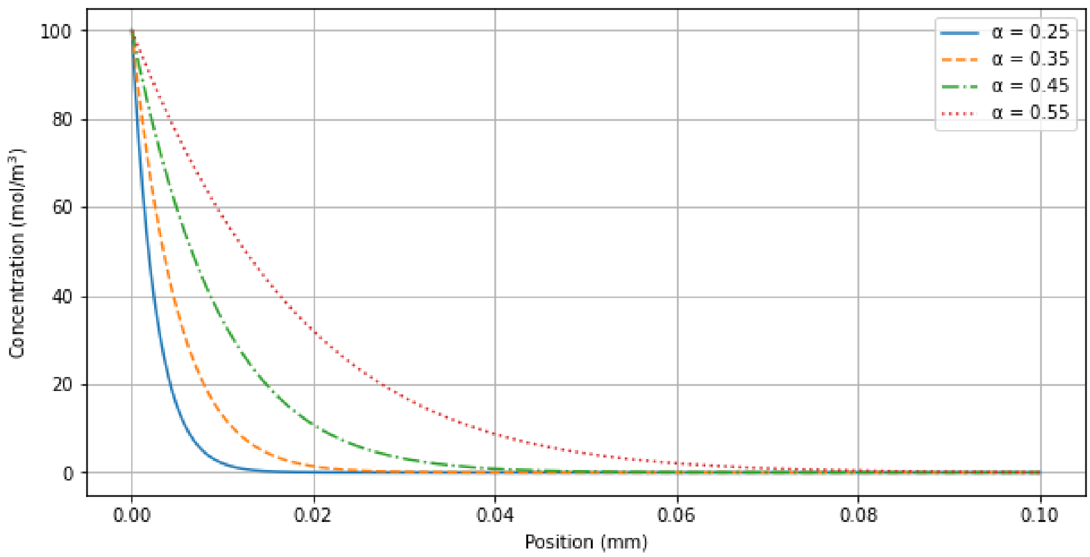

Figure 3. Concentration profiles in a smaller domain for lower α values at 48 h.

Another analysis was performed to see how the concentration for a single point evolves over the 48 hours for the fractional orders presented in Fig. 2. For the fixed point $x = 0.2\ mm$, Fig. 4 illustrates the relationship of concentration vs. time.

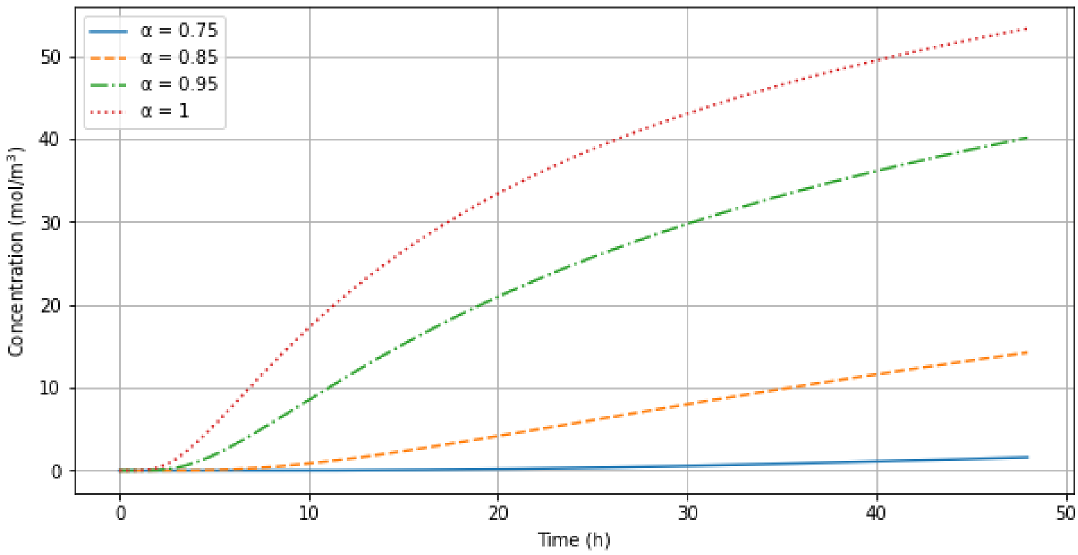

Figure 4. Concentration vs. time in $x = 0.2\ mm$ for different α fractional order.

The effect of the fractional order on the diffusion velocity is remarkable, as shown in Fig. 2 to 4. Table 1 summarizes the results, comparing the concentration values obtained at the point $x = 0.2\ mm$ in time $t = 48\ h$ and their percentage in relation to the ideal condition.

Table 1. Effects of the fractional order.

α **Order**	u **(mol/m³)**	u/u_{ideal} **(%)**
0.50	8.88E-09	1.66E-08
0.75	1.607	3.01
0.85	14.240	26.70
0.95	40.147	75.27
1	53.335	100.00

In this simplified study, the Caputo fractional operator represents an effective delay in the process and can realistically replicate the ideal case if necessary. For real data, a fine adjustment of the α order must be made, as the value can greatly affect the behavior of the diffusion.

4 Conclusions

This paper presents a first development of the solution of a FPDE using the Caputo operator with the FEM formulation for anomalous diffusion problems with classical boundary conditions. The problem that motivated the study is far from being fully represented, and the presence of advection terms and the dependence of the diffusion coefficient with space should be considered by treating the problem as a Fokker-Plank equation. The order of the fractional derivative capable of representing the real phenomenon of diffusion in polyamide still needs to be defined by appropriate experimental tests. However, the results provide a viable tool for further simulations in higher dimensions and tests with other fractional derivatives, which will be the next steps of this research.

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References

[1] F. A. Oliveira, R. M. S. Ferreira, L. C. Lapas and M. H. Vainstein, "*Anomalous Diffusion: A Basic Mechanism for the Evolution of Inhomogeneous Systems*". Frontiers in Physics, vol. 7, article 8, 2019.
[2] D. M. Tartakovsky and M. Dents, "*Diffusion in Porous Media: Phenomena and Mechanism*". Springer Nature B.V., Transport in Porous Media, 130, pp. 105–127, 2019.
[3] E. K. Lenzi, A. Somer, R. S. Zola, L. R. da Silva and M. K. Lenzi, "*Generalized Diffusion Equation: Solutions and Anomalous Diffusion"*. Fluids, vol. 8, article 34, 2023.
[4] I. Ali, N. Malik, B. Chanane, "*Fractional Diffusion Model for the Transport through Porous Media*". 5th International Conference on Porous Media and Their Applications in Science, Engineering, and Industry, 2014.
[5] Y. Luchko, "*Anomalous Diffusion Models and their Analysis*". Forum der Berliner Mathematischen Gesellschaft, 19, 53-85, 2011.
[6] A. A. Tateishi, H. V. Ribeiro, E. K. Lenzi, "*The Role of Fractional Time-derivative Operators on Anomalous Diffusion*". Frontiers in Physics, vol. 5, article 52, 2017.
[7] M. Concezzi and R. Spigler, "*Identifying the Fractional Order in Anomalous Diffusion Models from Real Data*". Fractal and Fractional, vol. 2, article 14, 2018.
[8] O. C. Zienkiewicz and R. L. Taylor, "*The Finite Element Method Volume 1: The Basis*". Butterworth-Heinemann, 5th Edition, 2000.
[9] M. Ciesielski and J. Leszezynski, "*Numerical Simulations of Anomalous Diffusion*". Computer Methods in Mechanics, Poland, 2003.
[10] R. M. Correa, J. A. M. Carrer, B. S. Solheid, J. Trevelyan, "*The Solution of the Anomalous Diffusion Equation by a Finite Element Method Formulation based on the Caputo Derivative*". Journal of the Brazilian Society of Mechanical Sciences and Engineering. 44, 250, 2022.
[11] M. R. S. Ammi, I. Jamiai, D. F. M. Torres, "*A Finite Element Approximation for a Class of Caputo Time-Fractional Diffusion Equations*". Computers and Mathematics with Applications, 78, pp. 1334-1344, 2019.
[12] M. Karimi, "*Diffusion in Polymer Solids and Solutions*". Mass Transfer in Chemical Engineering Processes, 2011.
[13] L. P. Razumovskii, V. S. Markin and G. Ye. Zaikov, "*Solubility and Diffusion Coefficient of Water in Aliphatic Polyamides*". Polymer Science U. S. S. R., vol. 27, no. 2, pp. 341-346, 1985.
[14] J. Crank, "*The Mathematics of Diffusion*". Second Edition, Oxford, 1975.